

# Assimilation of small scale soil moisture in a land surface model

Gabriëlle J.M. De Lannoy <sup>a</sup>, Niko E.C. Verhoest <sup>a</sup>, Valentijn R.N. Pauwels <sup>a</sup>, Paul R. Houser <sup>b</sup>

<sup>a</sup>Laboratory for Hydrology and Water Management, Ghent University, Coupure links 653,  
B-9000 Ghent, Belgium;

<sup>b</sup>George Mason University & Center for Research on Environment and Water, 4041 Powder  
Mill Road, Suite 302, Calverton, MD 20705-3106, USA

## ABSTRACT

Remote sensing offers a very interesting means to estimate the soil moisture state of a hydrological system. However, practical use for small scale agricultural applications is still limited. Ground truth data remain necessary to validate the inversion from the measured quantities to soil moisture content, to understand small scale processes in the horizontal plane, and to assess the distribution of water over a soil profile. Additionally, land surface models offer basic knowledge of the physical and physiological processes affecting the soil moisture state. A combination of both sources of information yields an optimal estimate of the system state and offers the best knowledge available to decision makers.

In this study, ground measurements of soil moisture in the Optimizing Production Inputs for Economic and Environmental Enhancement (OPE<sup>3</sup>) field (near Washington D.C.) of the United States Department of Agriculture (USDA) were assimilated into the Community Land Model (CLM2.0). Some practical problems that prevent optimal state estimation are discussed, such as the presence of bias in the model or observations, and the limited knowledge of the correlation structure of e.g. model error. Some case studies revealed that the influence of assimilation of upper layer soil moisture, as provided by remote sensing, improves the model results, but is not as persistent for profile estimation as assimilation of soil moisture in deeper layers.

**Keywords:** soil moisture, land surface model, assimilation

## 1. INTRODUCTION

Since soil moisture is an important state variable of the land surface system, the collection and analysis of soil moisture data at different spatial and temporal scales received a lot of attention. At the regional scale, soil moisture is known to interact with the atmosphere, to influence the climate and its change<sup>1</sup> and to have a controlling function in the hydrological cycle in general. At field scales, soil moisture has an impact on the generation of runoff and erosion, plant growth, and the chemical behavior of fertilizers, which is important to agriculture and environment. Soil moisture itself is influenced by a combination of atmospheric forcings, terrain features, texture, and vegetation.

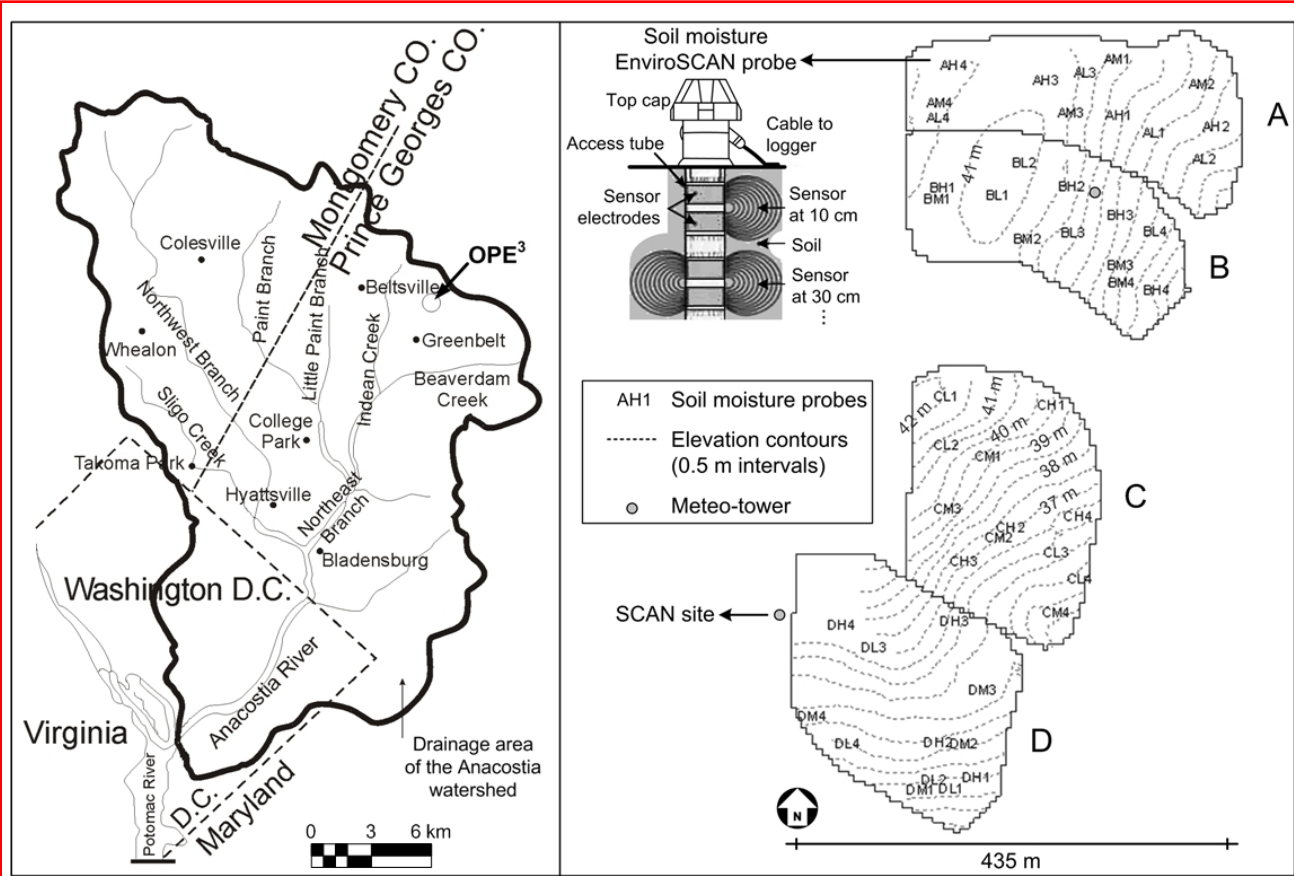
At the field scale, soil moisture values are generally obtained through ground measurements,<sup>2</sup> which are typically point measurements collected in 'representative' locations and at specific time instants. Detailed analysis of soil moisture patterns would require a dense network of observations, which is often impractical. Therefore, remote sensing offers a useful alternative to measuring soil moisture.<sup>3</sup> However, through these techniques, only the top layer soil moisture is captured and the current data rarely provide any information on detailed field variability. Furthermore, remote sensing data need to be validated with ground truth. Therefore, the collection and use of ground measurements remain a necessity.

In addition to the information from measurements, complementary information can be obtained from model results. It is through observed soil moisture patterns in space and time that natural processes can be understood and converted into physical laws, empirical relationships and land-surface model structures. Once a model

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Further author information:

E-mail: Gabrielle.DeLannoy@lid.kviv.be; Tel.: +32 (0)9 264 61 40; Fax: +32 (0)9 264 62 36



**Figure 1.** Left: Anacostia watershed and situation of the OPE<sup>3</sup> site. Right: OPE<sup>3</sup> field and location of soil moisture probes and some meteorological towers.

structure is set up, observations are needed for parameterization. Since the final model will never be perfect, observations are useful to update the state variables and parameters. State estimation by a combination of observations and model output is known as data assimilation. In case remote sensing data of top layer soil moisture only are available, model results will be necessary to complete the knowledge of the state of, and the processes in, the soil system and its environment. Based on this combined information, management practices can be adapted accordingly.

Since land-surface models are nonlinear, an interesting alternative to the (extended) Kalman filter<sup>4</sup> for state estimation is the ensemble Kalman filter.<sup>5</sup> First and second order statistics needed in the estimation procedure are calculated based on randomly sampled ensemble members. The problem with assimilation of data is that optimal results depend on the correctness of some assumptions concerning the statistics. Often these assumptions are violated in practice: the model or the observations contain biases, which are persistent non-zero mean errors and the structure of the errors is not known. Even multi-objective calibration, considering many different calibration measures and variables, cannot assure that model forecasts are unbiased for all variables. Observation bias is easier to remove through sensor calibration. However, for remotely sensed observations there is a higher risk of biases, because the inversion algorithm may contain shortcomings and the measurement circumstances are mostly not as well monitored as for in situ measurements. Ref. 6 discussed the need to estimate bias and developed a method to estimate the forecast bias and to correct the state separately, as discussed earlier by Ref. 7. This method is easy to implement and improves the results considerably.

## 2. DATA DESCRIPTION

### 2.1. OPE<sup>3</sup> field

The Optimizing Production Inputs for Economic and Environmental Enhancement (OPE<sup>3</sup>) project is an interdisciplinary research project which started in 1998. This project addresses major environmental and economic issues facing agriculture. The project is managed by the Beltsville Agricultural Research Center (BARC) - Agricultural Research Service (ARS) of the United States Department of Agriculture (USDA). For more information on this project, we refer to <http://hydrolab.arsusda.gov/ope3/>.

The project is conducted on a corn field of 21 ha, subdivided into 4 fields, each corresponding to a subwatershed of approximately 4 ha. The site is situated in Prince Georges County, Maryland, USA. The 4 subwatersheds are named A, B, C and D from North to South. The field is located in the Anacostia watershed (Figure 1), which is part of the Middle Potomac-Anacostia-Occoquan watershed, cataloged by the U.S. Geological Survey (USGS) under Hydrologic Unit Code 02070010. Water draining from the field feeds a wooded riparian wetland and first-order stream, Beaver Dam Creek, which subsequently drains into the Anacostia river, the Potomac river and the Chesapeake Bay.

The major geological formation in the area of the research site dates from the Cretaceous. Each of the subwatersheds of the OPE<sup>3</sup> field was formed by sandy fluvial deposits. The top soil can be described as sandy loam according to the USGS soil classification, with an average of  $15.62 \pm 1.63$  % clay,  $22.19 \pm 4.07$  % silt and  $62.17 \pm 5.56$  % sand. A clay lens is present under the entire site, varying from 0.9 m to 3.5 m below the soil surface.<sup>8</sup>

Concerning the land use over the last years, the field site itself has changed from an area with limited infrastructure, e.g. roads and little buildings, to an agricultural field. During summer, corn is grown on the OPE<sup>3</sup> field. The 4 subwatersheds are managed by the BARC-ARS of the USDA with different nutrient management practices for the 4 subwatersheds.

### 2.2. Soil moisture measurements

In each subwatershed of the OPE<sup>3</sup> field, 12 soil moisture probes have been installed (Figure 1) to independently determine how subsurface restricting layers, detected by ground penetrating radar (GPR), influence soil water dynamics.<sup>8</sup> Capacitance probes (EnviroSCAN, SENTEK Pty Ltd., South Australia) are used to measure volumetric water contents within a 10 cm radius from the sensor's center.<sup>9</sup> Since the site is sandy and receives over a meter of precipitation each year, neither the high soil surface area nor salts will be influencing the soil-water dielectrics. Consequently, the capacitance method is well suited to evaluate real-time soil water dynamics. The sampling interval is 10 minutes and for this study, data collected from May 1, 2001 to May 1, 2002 were analyzed. To compare data and model results in a further stage, a transformation was performed on the observations to change the aggregation time from 10 minutes to 1 hour by averaging. It should be indicated that the summer of 2001 was exceptionally wet.

The probes are named following a 3 digit system. The first letter represents the name of the subwatershed (A, B, C, D), the second letter (L, H, M) refers to the estimated infiltration rate at the point of installation (Low, High, Moderate) and the third digit (1, 2, 3, 4) discerns between the different probes of a specific infiltration regime. H-probes have sensors at 10 cm, 30 cm and 80 cm. L- and M-probes have sensors at 10 cm, 30 cm, 50 cm, 120 cm, 150 cm and 180 cm. L-probes have an additional sensor at 80 cm depth. During the study period, probes AL3, AL4, AM3, AM4, AH3, AH4, CL3, CL4, CM3, CM4, CH3 and CH4 were not operational because of technical defects (hit by lightning), causing 36 out of 48 probes to remain operational.

The spatial and temporal characteristics of the available data set of soil moisture are discussed in Ref. 10.

## 3. MODEL DESCRIPTION

The Community Land Model (CLM) is a global land surface model whose initial code was completed in 1998 by combining the best features of three existing modular land models: the Biosphere-Atmosphere Transfer Scheme (BATS,<sup>11</sup>), the Land Surface Model (LSM,<sup>12</sup>), and the model developed at the Institute of Atmospheric Physics

(IAP94,<sup>13</sup>) in Beijing. Ref. 14 reported some recent experiences from this CLM project. In this work, CLM2.0 was used in off-line mode, without any coupling to an atmospheric or climate model.

The CLM2.0 models biogeophysical and other processes over a predefined grid by calculating water and heat fluxes and states for every grid cell separately, without any interaction between cells. Each grid cell can be subdivided into several patches, containing one single land cover type: vegetation, bare soil, wetland, lake, urban and glacier. In this study, each grid cell was completely covered with vegetation. The vegetated fraction is further subdivided into patches of plant functional types. Each patch maintains its own prognostic variables. By default, all patches within a grid cell have the same (grid cell) soil texture, soil color, and corresponding physical properties and they respond to the same mean conditions (forcings) of the overlying atmospheric grid cell.

CLM2.0 has one vegetation layer, a user defined number (by default 10) of vertical soil layers, and up to 5 snow layers (depending on the snow depth). For this work, the choice for the depths of the nodes of the different soil layers was based on the depths of the soil moisture observations and the need for thin surface layers to assure numerical convergence. The depths of the different soil nodes were set to 2.5, 5, 10, 20, 30, 50, 80, 120, 150 and 180 cm depth. The model was integrated forward with a constant hourly time step.

#### 4. MULTI-OBJECTIVE MODEL CALIBRATION

The model runs were initiated on January 01, 2001. A calibration period of 1 month was chosen in September 2001 (from September 02, 2001 through October 01, 2001). In this period, observations showed no evidence of lateral flow, as could be observed for some preceding months. Including this phenomenon would result in parameters that try to compensate for structural model errors, since the model does not simulate horizontal water flow.

A purely random Monte Carlo (MC) search was performed to calibrate the CLM2.0 for soil moisture. Instead of multiple running (restarting) the CLM2.0 at identically the same grid cell, the subdivision of grids and patches was used to calculate MC realizations by simulating over all patches in space. Through this combination of grid cells and patches,  $15 \cdot 10^4$  MC simulations were generated, and from this collection of simulations, a best parameter set was extracted for each sensor.

A multi-objective<sup>15-17</sup> calibration procedure was developed, considering different measures of goodness-of-fit and different time series of soil moisture at the different depths in a profile. The misfit between the modeled initial state during the day of May 03, 2001 and the observations was penalized two orders of magnitude more (factor 100) than the misfit during September, to mimic the common practice of using observations as best initial guess for the initial conditions. Iterative sorting of the values for the different objective functions was performed and after each sort the worst patches were excluded for further competition, until a single best solution was obtained. The model runs with the calibrated parameter sets will be referred to as control run in the remainder of this paper.

#### 5. ENSEMBLE PREDICTION

CLM2.0 ensembles were generated by exploring the strong (assuming a perfect model and errors are due to bad initialization) as well as the weak (the model parameters and input are not assumed to be perfect) constraint approach. Different types of ensemble runs were performed: (1) perturbing initial states only, (2) perturbing parameters only, (3) perturbing forcings only, (4) perturbing parameters and initial states, and (5) perturbing parameters, initial states and forcings. Generation of ensemble members was performed by perturbation of parameters and initial states around the optimal mean found by calibration and around the observed values for the forcings. For this application, a grid cell was assigned to each sensor and the patches in it were used for the generation of ensemble members.

It was shown in Ref. 18 that the perfect model approach cannot be applied for bounded hydrological applications and that perturbation of parameters is a necessity to obtain a realistic assessment of the forecast error. Perturbation of forcings only captures more of the model uncertainty than perturbation of initial conditions only, but also causes a too limited spread in the ensembles. The generation of ensemble members through perturbation of the parameter set, found through calibration, does not necessarily result in ensembles that surround the

calibrated deterministic control run for soil moisture. This indicates that some parameter sets are not robust and not appropriate to perturb for ensemble generation: sometimes the resulting ensemble mean may not represent the best forecast or a priori state estimation. During periods of extreme drought or precipitation, the ensemble probability density function (pdf) deviates far from normality and the model behaves highly non-linear. For state estimation, the Kalman filter will only provide an optimal a posteriori/analysis estimate in the limited class of linear filters, since the underlying pdfs cannot be assumed to be Gaussian.

## 6. KALMAN FILTER

The Kalman filter (KF) calculates an optimal a posteriori/analysis state estimate  $\hat{\mathbf{x}}_i$  at time step  $i$ , based on the a priori/forecasted state estimate  $\hat{\mathbf{x}}_i^-$  and observations  $\mathbf{y}_i$ . The a priori state estimate is linked to the observations  $\mathbf{y}_i$  by the matrix  $\mathbf{H}_i$ :

$$\mathbf{y}_i = \mathbf{H}_i \mathbf{x}_i + \mathbf{v}_i \quad (1)$$

$\mathbf{v}_i$  is the the observation error, with  $E[\mathbf{v}_i] = 0$  and  $E[\mathbf{v}_i \mathbf{v}_i^T] = \mathbf{R}_i$ . The residual  $(\mathbf{y}_i - \mathbf{H}_i \hat{\mathbf{x}}_i^-)$  and the a priori state estimate are weighted by the Kalman gain  $\mathbf{K}_i$  as follows:

$$\hat{\mathbf{x}}_i = \hat{\mathbf{x}}_i^- + \mathbf{K}_i [\mathbf{y}_i - \mathbf{H}_i \hat{\mathbf{x}}_i^-] \quad (2)$$

The Kalman<sup>4</sup> gain  $\mathbf{K}_i$  is calculated as the ratio of the error covariance of the a priori estimate  $\mathbf{P}_i^-$  (related to the observations) to the error covariance of the residuals:

$$\mathbf{K}_i = \mathbf{P}_i^- \mathbf{H}_i^T [\mathbf{H}_i \mathbf{P}_i^- \mathbf{H}_i^T + \mathbf{R}_i]^{-1} \quad (3)$$

The KF explicitly propagates the error covariance matrices by an equation that is rather computational intensive and inaccurate for non-linear models. Ref. 19 used an ensemble of model trajectories (MC approach) to determine the error covariances directly from the spread of the states in an ensemble. The ensemble Kalman filter (EnKF) was used in this study.

### 6.1. System definition

The state vector consists of prognostic variables used in CLM2.0, i.e. canopy water, vegetation temperature, 10 layer soil temperature and 10 layer soil moisture. These variables are taken at 36 points (grid cells), resulting in a state vector of dimension  $n = 22 \times 36 = 792$ . The state is propagated in time by the CLM2.0, which does not need to be linearized for the EnKF. The input to force the model consists of meteorological variables, which are constant in space.

### 6.2. Interpolation matrix $\mathbf{H}$ , error statistics $\mathbf{P}$ and $\mathbf{R}$

Since the observations used for assimilation consist of direct measurements of state variables, i.e. soil moisture,  $\mathbf{H}$  contains only values of 0 and 1 and each row contains exactly one 1. Through ensemble generation as discussed above, it is not possible to determine any cross correlation between state errors in the horizontal for the CLM, since the model does not simulate lateral flow (only vertical). Therefore, neighbouring cells are not influenced by assimilation of soil moisture at any depth in any other cell and  $\mathbf{P}^-$  is made block diagonal, by removing spurious correlations.  $\mathbf{R}$  is diagonal, containing the variances of the errors for each observation, which are set to 0.0005 for soil moisture expressed in fractions (there is no cross correlation between the observation errors). Consequently,  $\mathbf{K}$  contains non-zero values for those elements only in the rows (22 rows out of 792) which correspond to the state variables that are directly related to an observation, causing that corrections are propagated over the profile only and not to neighbouring grid cells.

Through ensemble generation, information on the model error covariance is incorporated in  $\mathbf{P}_i$ . In this study, this information is only contained in the blocks around the diagonal elements, while no information of model error structure is available for the other elements. However, it can be included through external knowledge as explored by e.g. Ref. 20. Adaptive Kalman filtering also offers an interesting alternative to solve this problem and is subject to further research. In order to assess the second order statistics, it is important to assure correct estimates of first order statistics. However, it was found that the ensemble mean may sometimes deviate



considerably from the truth. Calibration could not remove all bias in the model results. If data were assimilated at a point where bias was present in the model results, this bias was included in the residual and possibly introduced bias in surrounding soil layers within a profile. This is illustrated in Figure 2, where assimilation of soil moisture at 80 cm depth causes extra bias for soil moisture at e.g. 30 cm depth. Bias (for soil moisture) in a layer cannot be removed by assimilation.

## 7. BIAS AWARENESS

### 7.1. Method

Ref. 7 presented a technique, known as the ‘separate-bias estimation’, where the estimation of the bias is essentially decoupled from the computation of the bias-blind estimate of the state. Ref. 6 discussed the link between the bias parameter estimation explained in the work of Ref. 7 and the estimation of the forecast bias  $\mathbf{b}_i^f$ . Forecast bias is defined as:

$$E[\mathbf{x}_i - \hat{\mathbf{x}}_i^-] = \mathbf{b}_i^f \quad (4)$$

with  $\mathbf{x}_i$  the true unbiased state and  $\hat{\mathbf{x}}_i^-$  the best a priori estimate, which is biased. The biased a posteriori state  $\hat{\mathbf{x}}_i$  is calculated by the unchanged equations for state estimation through Kalman filtering (see Eq. 2), and the bias is updated by another Kalman filter:

$$\hat{\mathbf{b}}_i^f = \hat{\mathbf{b}}_i^{f-} + \mathbf{K}_{bf,i}[\mathbf{y}_i - \mathbf{H}_i\hat{\mathbf{x}}_i^-] \quad (5)$$

with  $\hat{\mathbf{x}}_i^- = \hat{\mathbf{x}}_i^- + \hat{\mathbf{b}}_i^{f-}$ , and  $\hat{\mathbf{b}}_i^{f-}$  the estimate of the bias, which equals  $\hat{\mathbf{b}}_{i-1}^f$  for a persistence model. The blending matrix  $\mathbf{K}_{bf,i}$  is calculated by:

$$\mathbf{K}_{bf,i} = \mathbf{P}_{bf,i}^- \mathbf{H}_i^T [\mathbf{H}_i \mathbf{P}_{bf,i}^- \mathbf{H}_i^T + \mathbf{H}_i \tilde{\mathbf{P}}_{x,i}^- \mathbf{H}_i^T + \mathbf{R}_i]^{-1} \quad (6)$$

$\mathbf{P}_{bf,i}^-$  is the bias error covariance and  $\tilde{\mathbf{P}}_{x,i}^-$  the error covariance as calculated without awareness of bias. Ref. 6 proposed to calculate  $\tilde{\mathbf{P}}_i^-$  and  $\mathbf{P}_{bf,i}^-$  as a fraction of  $\mathbf{P}_{x,i}^-$ , the actual error covariance matrix:

$$\mathbf{P}_{bf,i}^- = \gamma \mathbf{P}_{x,i}^- \quad (7)$$

$$\tilde{\mathbf{P}}_{x,i}^- = (1 - \gamma) \mathbf{P}_{x,i}^- \quad (8)$$

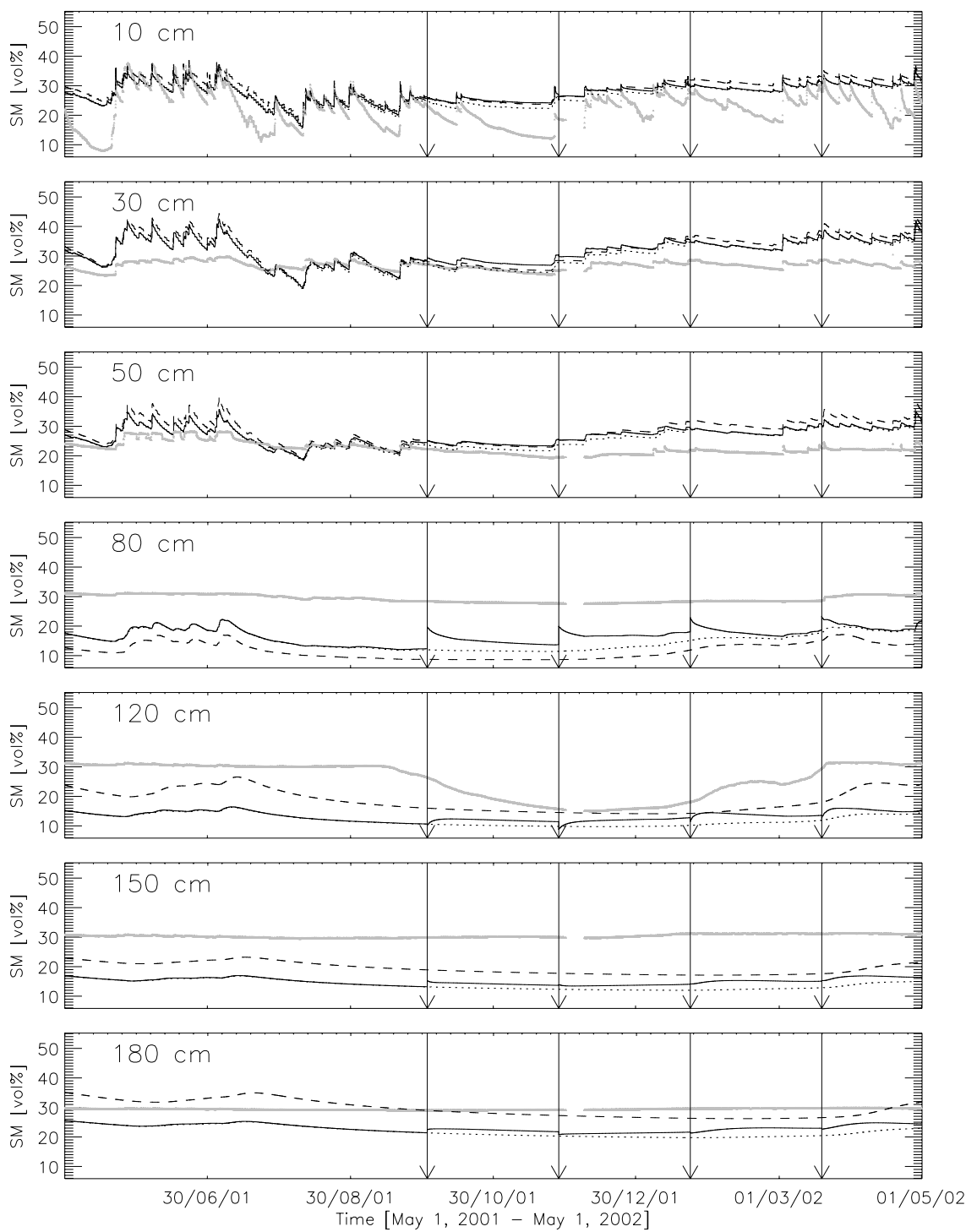
The parameter  $\gamma$  in the covariance model controls the stability of the bias estimates. It determines how much information in the observations is used to estimate the forecast bias and how much of uncertainty is left to random model error. Finally, the bias corrected state (not fed back into the model) is given by :

$$\hat{\mathbf{x}}_i = \hat{\mathbf{x}}_i^- + [\mathbf{I} - \tilde{\mathbf{K}}_{x,i} \mathbf{H}_i] \hat{\mathbf{b}}_i^f \quad (9)$$

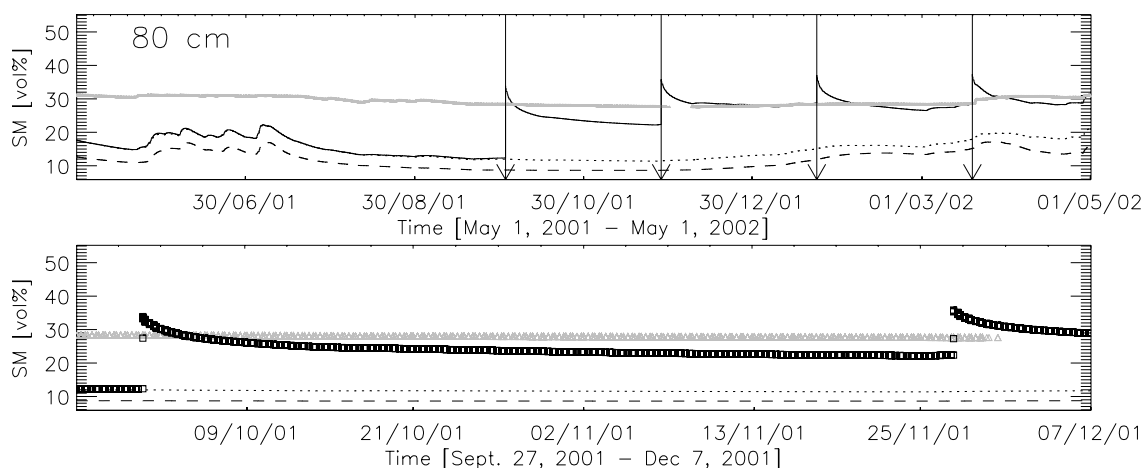
### 7.2. Results

Taking into account bias during assimilation was found to improve the overall model performance. However, the assumed persistence model for the bias propagation  $\hat{\mathbf{b}}_i^f = \hat{\mathbf{b}}_{i-1}^f$  should be relaxed. After assimilation, the influence of the ‘biased’ state update is still clear and hence an additional bias term causes overshoot in the predicted bias-corrected state estimate  $\hat{\mathbf{x}}_i^- = \hat{\mathbf{x}}_i^- + \hat{\mathbf{b}}_i^f$  as long as the influence of the ‘biased’ state update is present. This is illustrated in Figure 3. Further, for this study there is no evidence that  $\mathbf{P}_{bf,i}^-$  would be proportional to  $\tilde{\mathbf{P}}_{x,i}^-$  and more accurate covariance models will definitely further enhance the filter’s performance.

Several assimilation scenarios were set up to study the influence of the choice of assimilation frequency and depth on the overall profile estimation. The results revealed that observations are best collected and assimilated spread in time, instead of close together. Further it was found that top layer soil moisture is less effective for assimilation than soil moisture at deeper layers, which has a more persisting influence. It is expected that further improved results will be obtained from adaptive Kalman filtering.



**Figure 2.** Soil moisture (SM) time series at DL3 with observations (gray), the control run (black dashed), the ensemble mean run (black dotted), and the ensemble KF run (black line) with filtering of soil moisture in the 80 cm of DL3 at a low frequency of assimilation. The arrows indicate the filtering time steps.



**Figure 3.** Upper plot: similar to Fig. 2, but only at 80 cm depth and with inclusion of bias estimation ( $\gamma = 0.5$ ). Lower plot: the zoom of the first 2 assimilation steps illustrates that the persistence bias model causes an overshoot in the predicted bias-corrected state (black squares~black line in upper plot) as long as the influence of the ‘biased’ state update is present.

## 8. CONCLUSIONS

The CLM2.0 was used to represent the the system of the OPE<sup>3</sup> field of the USDA-BARC. The model was calibrated by soil moisture observations in a multi-objective framework to limit model random error and forecast bias. Ensemble predictions were generated by perturbation of initial states, parameters and forcings. It was found that the ensemble mean, which serves as a priori estimate for state estimation, was not necessary closer to the truth than the control run and that sometimes an extra bias worsened the results. An update of the a priori state estimation through inclusion of observational data did improve the results, but not in case the corresponding model results were biased. A bias-aware ensemble Kalman filter was able to improve the results considerably. Some case studies have shown that it is best to assimilate observations spread over time and preferably not the surface soil moisture, since its influence is only limited in time. Further research will include the estimation of the model error covariance to compensate for model deficiencies in the CLM2.0.

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